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The Application of Surface Dislocation Theory to the F.c.c.–B.c.c. Interface

BY K. M. KNOWLES

University of Oxford, Department of Metallurgy and Science of Materials, Parks Road, Oxford OX1 3PH, England

AND D. A. SMITH

IBM Corporation, T. J. Watson Research Center, Yorktown Heights, NY 10598, *USA*

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Abstract

The formal theory of surface dislocations has been applied to the f.c.c.–b.c.c. interfaces defined by $(111)_F \| (110)_B$. With the Bain correspondence between the two lattices, various theoretical models and experimental results on these interfaces have been analyzed. The results of the analysis suggest that preferred interface orientations can be explained on the basis that they are those of minimum or near-minimum Burgers-vector contents. This concept leads to an improved criterion for comparing the elastic component of interfacial energies. The limitations of geometrical models for predicting low-energy interfaces are discussed.

1. Introduction

In this paper, we describe f.c.c.–b.c.c. boundaries in terms of the formal geometrical theory of surface dislocations (Bilby, Bullough & de Grinberg, 1964), of which the 0-lattice theory (Bollmann, 1970) may be considered to be a quantized version (Christian, 1976). We also discuss the extent to which criteria such as 'best fit' are successful in predicting observed interface orientations. Particular emphasis is given to experimental results from the copper–chromium age-hardening alloy system (Hall, Aaronson & Kinsman, 1972; Weatherly, Humble & Borland, 1979) for which the theory of Bollmann (1974) is appropriate when the chromium-rich b.c.c. precipitates have a Nishiyama–Wasserman (N–W) orientation relationship (Nishiyama, 1934) with the f.c.c. matrix. We start by discussing the formal theory of surface dislocations before analyzing the interface models of Bruce & Jaeger (1978), Hall *et al.* (1972) and Rigsbee & Aaronson (1979*a*,*b*).

2. The model of a general f.c.c.–b.c.c. interface

The Burgers vector content **B** of an interface between two phases designated by the subscripts + and − can be defined through the formula

$$\mathbf{B} = (\mathbf{S}_+^{-1} - \mathbf{S}_-^{-1})\,\mathbf{p}, \tag{1}$$

where **p** is a vector in the interface and $\mathbf{S}_+$ and $\mathbf{S}_-$ are the deformations carrying the reference lattice, in which **B** and **p** are expressed in the final orientations of the (+) and (−) lattices respectively. If we choose the (+) lattice to be the reference lattice, which is transformed into the (−) lattice by the deformation **S**, the formula becomes

$$\mathbf{B} = (\mathbf{I} - \mathbf{S}^{-1})\,\mathbf{p}. \tag{2}$$

If we suppose that the misfit in the interface defined by (2) is accommodated by a network of i parallel sets of dislocations of Burgers vectors $\mathbf{b}_i$, line vector $\boldsymbol{\xi}_i$ and spacing d_i, we can rewrite (2) in the form (Sargent & Purdy, 1975)

$$\mathbf{B} = \sum_i (\mathbf{N}_i . \mathbf{p})\,\mathbf{b}_i = (\mathbf{I} - \mathbf{S}^{-1})\,\mathbf{p}, \tag{3}$$

where

$$\mathbf{N}_i = \frac{\mathbf{v} \times \boldsymbol{\xi}_i}{d_i}$$

and **v** is a unit vector normal to the boundary.

The form of (2) demonstrates that if **p** is fixed in length and none of the three eigenvalues of **S** is equal to unity, then the locus of all points **B** defined through the equation is the surface of an ellipsoid. The principal axes of the ellipsoid can be determined by application of Lagrange multipliers to the function

$$f(\mathbf{p}) = \sum_i B_i B_i \tag{4}$$

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subject to the condition

$$g(\mathbf{p}) = 1 - \sum_i p_i p_i = 0. \tag{5}$$

If we confine $\mathbf{p}$ to the boundary with normal ν, then the condition

$$h(\mathbf{p}) = \sum_i p_i \nu_i = 0 \tag{6}$$

together with (5) determines the principal axes of the ellipse describing the net Burgers-vector content crossing all unit vectors $\mathbf{p}$ in ν. For a given $\mathbf{S}$, the interface with the lowest values of the principal axes of this ellipse can be said to be the interface with minimum net Burgers-vector content and therefore of best fit between the two lattices.

We note, however, that (1)–(3) do not give a unique specification for the misfit between two phases, since each possible deformation $\mathbf{S}$ relating the (+) and (−) lattices will yield a different value of $\mathbf{B}$ (Bilby *et al.*, 1964; Bollmann, 1970; Christian, 1976). Thus, to obtain a 'correct' dislocation description of an interface, an additional criterion is needed to select $\mathbf{S}$. Bollmann (1970) suggests that $\mathbf{S}$ is chosen so that the determinant $|\mathbf{I} - \mathbf{S}^{-1}|$ is as small as possible, whilst another criterion is to determine the least maximum modulus of $|\mathbf{B}|$ (Bilby *et al.*, 1964; Christian, 1976). However, both these criteria have their limitations (Christian & Crocker, 1980) and the choice of $\mathbf{S}$ is usually made by appealing to the particular physical situation. For martensitic transformations, $\mathbf{S}$ is obtained from an assumed lattice correspondence between the parent and product phases. In the case of grain boundaries close to coincidence-site-lattice (CSL) orientations, experimental observations of grain boundary dislocation networks can be explained if the dislocations are DSC dislocations of the nearby CSL with $\mathbf{S}$ being a rotation matrix describing the deviation away from the CSL (Clarebrough & Forwood, 1980*a*,*b*). For more general phase boundaries the concept of a near coincidence between two non-primitive cells $M1$ and $M2$ belonging to the two lattices has been used (Bonnet & Durand, 1975; Bonnet & Cousineau, 1977). For the f.c.c.–b.c.c. interface following Bollmann (1974) we will use the Bain correspondence (Bain, 1924) commonly used in the phenomenological theory of martensitic transformations. This may be expressed in matrix notation as follows:

$$({}_B C_F) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 1 & 0 \\ -1 & 1 & 0 \end{bmatrix},$$

where the prefix B and suffix F denote the b.c.c. and f.c.c. phases respectively and ${}_B C_F$ is the correspondence matrix in the extended notation of Mackenzie & Bowles (1954). Thus, the unit vectors of the f.c.c. cell, $\frac{1}{2}[10\bar{1}]_F$, $\frac{1}{2}[01\bar{1}]_F$ and $\frac{1}{2}[110]_F$ correspond to the unit vectors $\frac{1}{2}[\bar{1}\,1\,\bar{1}]_B$, $\frac{1}{2}[\bar{1}11]_B$ and $[010]_B$ of the b.c.c. cell of Bollmann [Fig. 1 of Bollmann (1974)]. The deformation $({}_F S_F)$ carrying the f.c.c. lattice into the b.c.c. lattice may be written

$$({}_F S_F) = ({}_F T_B)({}_B C_F), \tag{7}$$

where $({}_F T_B)$ relates the components of any vector $\mathbf{x}$ referred to the B lattice to the components referred to the F lattice (Mackenzie & Bowles, 1954). We choose an orthonormal set of coordinates such that

$$\begin{aligned} \mathbf{x}_O &\| [11\bar{2}]_F \| [\bar{1}10]_B \\ \mathbf{y}_O &\| [\bar{1}10]_F \| [0001]_B \\ \mathbf{z}_O &\| [111]_F \| [110]_B, \end{aligned} \tag{8}$$

i.e. the f.c.c. and b.c.c. phases have a N–W orientation relationship. Transformation of (2) and (7) to the orthonormal set denoted by the subscript O defined in (8) leads to

$$(oSo) = (oT_B)({}_B C_F)({}_F To)$$

and

$$\mathbf{B}_O = [\mathbf{I} - (oSo)^{-1}]\,\mathbf{p}_O. \tag{9}$$

Hence, for lattice parameters a_B, a_F of the b.c.c. and f.c.c. phases, we obtain

$$(oSo) = \frac{a_B}{a_F} \begin{bmatrix} \sqrt{12}/3 & 0 & \sqrt{6}/6 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{6}/2 \end{bmatrix}, \tag{10}$$

which is the same as equation (6) of Bollmann (1974) for $a_F/a_B = 1{\cdot}254$. Relative rotation of the B and F lattices away from the N–W orientation relationship can be modelled by pre-multiplying (oSo) by a rotation matrix $\mathbf{R}$.

3. Applications

3.1. *Epitaxial* (111) *f.c.c.*–(110) *b.c.c. interfaces*

In a recent investigation of the deposition of f.c.c. metals on (110) b.c.c. metal substrates and of b.c.c. metals on (111) f.c.c. metal substrates, Bruce & Jaeger (1978) found that the metals epitaxed in either a N–W orientation relationship or in a Kurdjumov–Sachs (K–S) (Kurdjumov & Sachs, 1930) orientation relationship, depending on the ratio of the bulk atomic diameters of the deposit and substrate metals. They simulated (111) f.c.c.$\|$(110) b.c.c. interfaces by taking nets of discs representing atoms in the two planes and

superimposing them in the two orientations, N–W and K–S, *i.e.* they made moiré models similar to those used by Bollmann (1970). They then explained their results by showing that areas where the discs in the two nets coincided were more elongated in the alignment adopted. It is a straightforward exercise to explain their experimental results with the methods outlined in § 2.

If we consider the N–W orientation first, the principal axes of the ellipse describing the misfit between the f.c.c. and b.c.c. phases in the (111) f.c.c.$\|$(110) b.c.c. interface plane are

$$\mathbf{B}_1 = \left(1 - \frac{\sqrt{3}}{2}\frac{a_F}{a_B}\right)\begin{bmatrix}1\\0\\0\end{bmatrix} \text{ along } \mathbf{p}_1 = \begin{bmatrix}1\\0\\0\end{bmatrix}$$

and

$$\mathbf{B}_2 = \left(1 - \frac{1}{\sqrt{2}}\frac{a_F}{a_B}\right)\begin{bmatrix}0\\1\\0\end{bmatrix} \text{ along } \mathbf{p}_2 = \begin{bmatrix}0\\1\\0\end{bmatrix} \qquad (11)$$

in the orthonormal basis in the f.c.c. lattice from (4)–(6), (8) and (9). We note that the net Burgers vector in the b.c.c. lattice is given in the orthonormal basis by

$$\mathbf{B}'_O = \mathbf{S}\mathbf{B}_O = [(oSo) - \mathbf{I}]\,\mathbf{p}_O, \qquad (12)$$

so, in general, the principal axes $\mathbf{B}'_1$ and $\mathbf{B}'_2$ will be different from $\mathbf{B}_1$ and $\mathbf{B}_2$ in both magnitude and direction. However, the angular differences between $\mathbf{B}_1$ and $\mathbf{B}'_1$, $\mathbf{B}_2$ and $\mathbf{B}'_2$, $\mathbf{p}_1$ and $\mathbf{p}'_1$, and $\mathbf{p}_2$ and $\mathbf{p}'_2$ are small for the deformation S derived here for the range of lattice parameters of interest. Thus, for the N–W orientations, for example, $\mathbf{B}_1\|\mathbf{B}'_1$, $\mathbf{B}_2\|\mathbf{B}'_2$, $\mathbf{p}_1\|\mathbf{p}'_1$ and $\mathbf{p}_2\|\mathbf{p}'_2$, but

$$|\mathbf{B}'_1| = \left(\frac{2}{\sqrt{3}}\frac{a_B}{a_F} - 1\right)$$

and

$$|\mathbf{B}'_2| = \left(\sqrt{2}\frac{a_B}{a_F} - 1\right).$$

We will therefore only consider $\mathbf{B}_1$, $\mathbf{B}_2$, $\mathbf{p}_1$ and $\mathbf{p}_2$ in this treatment.

Equation (11) shows that the misfit between the f.c.c. and b.c.c. lattices can be fully relieved in a purely formal sense by a rectangular array of edge dislocations with Burgers vectors parallel to $[11\bar{2}]_F$ and $[\bar{1}10]_F$, the spacings of the arrays being inversely proportional to $|\mathbf{B}_1|$ and $|\mathbf{B}_2|$ respectively. In particular, for a_F/a_B corresponding to the nets of Bruce & Jaeger (1978), we obtain

(*a*) $a_F/a_B = 1{\cdot}113$ $\rho = 1{\cdot}100$ $|\mathbf{B}_1| = 0{\cdot}036$, $|\mathbf{B}_2| = 0{\cdot}213$

(*b*) $a_F/a_B = 1{\cdot}291$ $\rho = 0{\cdot}949$ $|\mathbf{B}_1| = 0{\cdot}118$, $|\mathbf{B}_2| = 0{\cdot}087$

(*c*) $a_F/a_B = 1{\cdot}422$ $\rho = 0{\cdot}861$ $|\mathbf{B}_1| = 0{\cdot}006$, $|\mathbf{B}_2| = 0{\cdot}231$,

where $\rho = d_0$ b.c.c./d_0 f.c.c., the ratio of the bulk atomic diameters, and is related to a_F/a_B by $\rho = \sqrt{3}a_B/\sqrt{2}a_F$. Thus, in (*a*), the greater part of the misfit can be accommodated by a single array of dislocations with $\mathbf{B}\|[\bar{1}10]_F$ along $\boldsymbol{\xi} = [11\bar{2}]_F$ and, in (*c*), by another single array with $\mathbf{B}\|[11\bar{2}]_F$ along $\boldsymbol{\xi} = [\bar{1}10]_F$. In (*b*), the misfit is formally relieved by approximately equal dislocation densities in both arrays. The lozenge-shaped unfavorable areas, clearly apparent in the superimposed nets for case (*b*), where $|\mathbf{B}_1|$ and $|\mathbf{B}_2|$ are comparable, and less well defined for (*a*) and (*c*), have areas proportional to $(|\mathbf{B}_1||\mathbf{B}_2|)^{-1}$. Fig. 1 shows the superposition of nets representing the atoms in the $(111)_F\|(110)_B$ planes for $a_F/a_B = 1{\cdot}291$, case (*b*). Along $[11\bar{2}]_F\|[1\bar{1}0]_B$ there are $n = 1/|\mathbf{B}_1| \sim 8{\cdot}5$ f.c.c. atoms for every $(n+1)$ b.c.c. atoms whilst along $[1\bar{1}0]_F\|[001]_B$ there are $m = 1/|\mathbf{B}_2| \sim 11{\cdot}5$ f.c.c. atoms for every $(m-1)$ b.c.c. atoms. The areas of the lozenges in Fig. 1 are therefore

$$\left(n\frac{\sqrt{6}}{2}a_F\right)\left(m\frac{\sqrt{2}}{2}a_F\right) \equiv (m-1)\,a_B(n+1)\sqrt{2}a_B,$$

i.e. the area of the lozenge-shaped unfavorable regions, where the symbols representing the deposits and substrates are close enough to one another to give a dark region, is proportional to $(|\mathbf{B}_1|\,|\mathbf{B}_2|)^{-1}$. This result

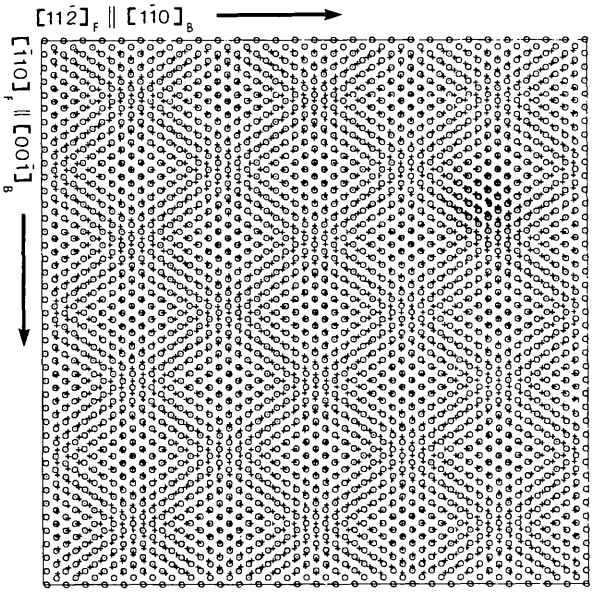

Fig. 1. Superposition of nets representing atoms in $(111)_F\|(110)_B$ planes for $a_F/a_B = 1{\cdot}291$. The atoms in the b.c.c. planes are represented by circles and those in the f.c.c. planes by crosses.

is valid for the general case, where the principal axes $\mathbf{B}_1$, $\mathbf{B}_2$, $\mathbf{p}_1$ and $\mathbf{p}_2$ are irrational directions (as in the K–S epitaxial orientation described below).

To obtain a K–S orientation relationship, we can rotate the b.c.c. lattice relative to the f.c.c. lattice by an angle $\theta = \cos^{-1}[(\sqrt{6} + 1)/2\sqrt{3}] \sim 5{\cdot}26°$ about $\mathbf{z}_O \| [111]_F \| [110]_B$, so making $[10\bar{1}]_F \| [\bar{1}1\bar{1}]_B$ and $[1\bar{2}1]_F \| [1\bar{1}\bar{2}]_B$. Table 1 shows values of $\mathbf{B}_1$ and $\mathbf{B}_2$ describing the misfit in the $(111)_F \| (110)_B$ interface plane along the directions $\mathbf{p}_1$ and $\mathbf{p}_2$ calculated with (2). The table shows that the K–S orientation nets of Bruce & Jaeger (1978) can also be explained by surface dislocation theory; for example, for $a_F/a_B = 1{\cdot}291$ and $\rho = 0{\cdot}949$, $|\mathbf{B}_1|$ and $|\mathbf{B}_2|$ are 0·009 and 0·196 respectively, with $\mathbf{p}_1$, the direction of best fit, being 44·2° away from $[\bar{1}10]_F$, and 15·8° from $[10\bar{1}]_F$ and can be identified as the direction of parallel fringes in Fig. 7(*c*) of Bruce & Jaeger (1978). The direction of worst fit in this analysis, $\mathbf{p}_2$, is necessarily perpendicular to $\mathbf{p}_1$. Thus, we can rapidly reach the same conclusions as Bruce & Jaeger, that areas where discs in the two nets coincide are more elongated in the adopted alignment, and to some extent justify and clarify their procedure with surface dislocation analysis, without the necessity of going through the procedure of superimposing nets, *i.e.* of producing moiré models of the interfaces.

3.2. *Partially coherent f.c.c.–b.c.c. boundaries*

In their study of chromium-rich b.c.c. precipitates in a f.c.c. matrix of a Cu–0·33 wt% Cr alloy, Hall, Aaronson & Kinsman (1972) observed irrational habit planes with orientation relationships varying from N–W to K–S. They found that most of their habit planes could be explained by modeling them as sequences of steps whose broad faces were formed by $(111)_F \| (110)_B$. The area of each step was restricted by the requirement that it was a region of good fit between the lattices. This model has been developed further by Rigsbee & Aaronson (1979*a*) for a wide range of a_F/a_B. It is again a straightforward exercise to obtain the results of their models with surface dislocation theory and demonstrate that their predicted interfaces are those with minimum net Burgers-vector content for the Bain correspondence between the f.c.c. and b.c.c. lattices and a given orientation relationship.

Table 1. *Kurdjumov–Sachs orientation relationship*

a_F,a_B are the lattice parameters of the f.c.c. and b.c.c. phases, respectively; $\rho = d_0$ b.c.c./d_0 f.c.c., the ratio of the bulk atomic diameters; $\mathbf{B}_1$,$\mathbf{B}_2$ are the principal axes of the ellipse describing the misfit between the two lattices in the $(111)_F \| (110)_B$ interface plane, referred to the orthonormal basis O; $\mathbf{p}_1$,$\mathbf{p}_2$ are the unit vectors related to $\mathbf{B}_1$ and $\mathbf{B}_2$ through equation (9) in the text.

a_F/a_B	ρ	$\mathbf{B}_1$	$\mathbf{B}_2$	$\mathbf{p}_1$	$\mathbf{p}_2$
		0·05958	−0·07672	0·97278	0·23171
1·113	1·100	0·02012	0·22715	−0·23171	0·97278
		0·00000	0·00000	0·00000	0·00000
		0·00550	−0·15276	−0·69733	0·71675
1·291	0·949	0·00680	0·12347	0·71675	0·69733
		0·00000	0·00000	0·00000	0·00000
		−0·01269	−0·25262	−0·40126	0·91597
1·422	0·861	−0·03818	0·08400	0·91597	0·40126
		0·00000	0·00000	0·00000	0·00000

Table 2 shows the principal axes of the **B** ellipsoid describing the misfit between the two lattices and the corresponding directions **p** defined in (2), in the f.c.c. reference lattice for $a_F/a_B = 1{\cdot}253$ and θ, the angular rotation away from N–W, having values of 0, 2 and 5·26°. Thus, for the N–W orientation, the interface containing $\mathbf{p}_1$ and $\mathbf{p}_2$ is that with the minimum net Burgers-vector content, *i.e.* $(0{\cdot}469, 0{\cdot}469, 0{\cdot}748)_F$, which is 1·8° away from $(223)_F$, 1·2° away from $(335)_F$ and 13·2° away from $(111)_F$. Similarly for the K–S orientation, the interface with the minimum net Burgers-vector content is $(0{\cdot}648, 0{\cdot}229, 0{\cdot}726)_F$, which is 22·2° away from $(111)_F$ and 3·16° away from $(313)_F$. Inspection of Fig. 11 of Rigsbee & Aaronson (1979*a*) shows that these interfaces are the *O–B* interfaces of Rigsbee & Aaronson, which give better agreement with the experimental results of Hall, Aaronson & Kinsman (1972) than the Rigsbee & Aaronson *O–A* interfaces, which will have far greater misfits to accommodate than the *O–B* interfaces. The same comment also applies to the interfaces with triatomic structural ledges stepping in the direction opposite to the ones producing the *O–A* and *O–B* interfaces; in fact, these latter interfaces will in general have a higher dislocation content than the $(111)_F \| (110)_B$ interfaces for a given orientation relationship. For example, in the N–W orientation, the interface predicted with the inverse rotated triatomic ledges is $(0{\cdot}655, 0{\cdot}655, 0{\cdot}376)_F$ which has values of 0·114 and 0·166 for the moduli of the principal axes of the **B** ellipsoid, compared with 0·085 and 0·114 for $(111)_F \| (110)_B$ and 0·005 and 0·114 for the interface with minimum net Burgers-vector content.

The experimental results of Rigsbee & Aaronson (1979*b*) suggest that the observed interfaces are indeed near those of minimum net Burgers-vector content, but have the deviation away from the $(111)_F \| (110)_B$ interface orientation made by structural triatomic ledges, with the atomic habit plane remaining $(111)_F \| (110)_B$. That the dislocations in the $(111)_F \| (110)_B$ interfaces are observed to have a Burgers vector lying in the interface is of course consistent with the surface dislocation analysis from inspection of equation (10) and the required form of any rotation matrix **R** to keep $(111)_F \| (110)_B$. These dislocations are sessile with respect to glide out of the interface.

Table 2. *Principal axes of the* **B** *ellipsoid and the corresponding* **p** *vectors for* $a_F/a_B = 1{\cdot}253$ *in the basis of the f.c.c. phase*

φ (°)	$\mathbf{B}_1$	$\mathbf{B}_2$	$\mathbf{B}_3$	$\mathbf{p}_1$	$\mathbf{p}_2$	$\mathbf{p}_3$	$\lvert B_1\rvert, \lvert B_2\rvert \lvert B_3\rvert$
	0·00317	−0·08061	0·13873	−0·52926	−0·70711	0·46892	0·00528
0 (N–W)	0·00317	0·08061	0·13873	−0·52926	0·70711	0·46892	0·11400
	0·00278	0·00000	−0·31637	0·66315	0·00000	0·74848	0·37227
	0·00259	0·08236	0·15407	−0·67987	0·48803	0·54736	0·00447
2	0·00278	−0·08288	0·12500	0·31668	−0·86860	0·38111	0·11707
	0·00235	0·00733	−0·31768	−0·66143	0·08577	0·74509	0·37455
	0·00035	0·09130	0·18229	−0·75293	0·11370	0·64820	0·00062
5·26 (K–S)	0·00040	−0·09609	0·10600	0·05062	−0·97204	0·22930	0·13403
	0·00032	0·01985	−0·32528	0·65615	0·20546	0·72612	0·38765

3.3. *Growth axis directions in* Cu–Cr

In a detailed study of precipitation of a chromium-rich b.c.c. phase in the f.c.c. matrix of a Cu–0·55 wt% Cr alloy, Weatherly, Humble & Borland (1979) found that the orientation relationship between their needle precipitates and f.c.c. matrix was within ±0·5° of K–S.

The predominant growth direction lay 7–9° from the $[0\bar{1}1]_F$ pole on the $(111)_F$ great circle, the nearest rational direction being either $[\bar{1}\bar{5}6]_F$ or $[\bar{1}\bar{6}7]_F$, corresponding to $[3\bar{3}4]_B$. The strain-field contrast effects around the needle were shown to have the same character as that of a dislocation dipole, to a first approximation, with the displacement vector of $[1\bar{5}4]_F$ and the Burgers vector associated with the dipole $\mathbf{b} = \frac{5}{4}[1\bar{5}4]_F$, for a needle axis direction of $[6\bar{1}\bar{5}]_F$.

Table 3 shows the application of surface dislocation analysis to this problem for $a_F/a_B = 1{\cdot}253$ and for orientations of K–S and ±0·25° away from K–S. Changing a_F/a_B to 1·252 or 1·254 does not significantly change the results of the calculations, which are, however, sensitive to angular changes within the quoted experimental error of Weatherly *et al.* (1979). This analysis clearly suggests that the growth axis direction of the chromium-rich needles is, as suggested (Weatherly *et al.*), to within the quoted error of ±2° in the stereographic analysis, the direction of best fit between the two lattices in the $(111)_F \| (110)_B$ plane. Furthermore, the direction of the Burgers vector of the dislocations crossing this direction is within 1–2° of the Burgers vector deduced from the analysis of Weatherly *et al.* for the exact K–S orientation and ±0·25° away from K–S; the magnitude of **B** is very sensitive to the orientation relationship. For the K–S orientation, the net Burgers vector along the chromium-rich needle considered by Weatherly *et al.* would be about $\mathbf{b} = 5/2[1\bar{5}4]$, and the strain field contrast could arise from the very slight mismatch along the needle axis.

As Table 2 shows, the direction of best fit irrespective of plane for the K–S orientation is also very close to the experimentally determined growth axis (3·3° away from $[7\bar{1}\bar{6}]_F$) and the fit along this direction is nearly perfect. In this case, the strain contrast would arise from the misfit in the plane of the particle cross section and the displacements **B** will lie in the $(111)_F$ plane to within a few degrees for all directions in this plane. There will therefore necessarily be a direction in the plane of cross section along which **B** is approximately $\| [1\bar{5}4]_F$, as there will be equally for the case where the growth axis is assumed to lie in the $(111)_F \| (110)_B$ plane above, from the form of **S**. This is consistent with the analysis of Weatherly *et al.* (1979). However, since the misfit in the plane of cross section is necessarily formally fully relieved by at least two arrays of dislocations, as in the two-consecutive-shears model of Kurdjumov & Sachs (1930), the limitations of associating a dislocation dipole character with these arrays have to be recognised (Weatherly *et al.*, 1979).

Table 3. *Directions of best fit* $\mathbf{p}_1$ *and corresponding Burgers-vector contents* $\mathbf{B}_1$ *in the* $(111)_F \| (110)_B$ *plane at and near the K–S orientation relationship in the basis of the f.c.c. phase for* $a_F/a_B = 1{\cdot}253$

φ (°)	$\mathbf{p}_1$	$\mathbf{B}_1$
	0·74911	0·00121
5·26	−0·09327	−0·00562
(K–S)	−0·65584	0·00441
	0·74891	0·00192
5·0	−0·09277	−0·00911
	−0·65614	0·00719
	0·74919	0·00055
5·5	−0·09346	−0·00250
	−0·65573	0·00195

Note: At the K–S orientation relationship $[10\bar{1}]_F \| [\bar{1}1\bar{1}]_B$ and $[1\bar{2}1]_F \| [1\bar{1}\bar{2}]_B$ for the case in the above table.

4. Discussion

4.1. *Geometrical predictions of phase boundary energies*

The results of the surface dislocation analysis presented here suggest that the concept of minimization of the net Burgers-vector content can be usefully applied to f.c.c.–b.c.c. interfaces to determine

possible favored interface planes, orientation relationships or growth axes. However, it is important to recognize that the surface dislocation model, as well as other geometric models, is at best semi-quantitative in terms of predicting likely interface planes and interfacial structure (Van der Merwe, 1974). No account is taken of chemical contributions to the interfacial energy and the correlation between a small value of $|\mathbf{B}|$ and a small elastic energy depends on the physical reality of the dislocations which are postulated only mathematically in the surface dislocation analysis. In spite of these limitations it is still pertinent to compare our analysis with other geometrical analyses which have been suggested as a guide to boundary energies (Bollmann, 1970; Bollmann & Nissen, 1968; Ecob & Ralph, 1980; Perio, Bacmann, Suery & Eberhardt, 1977).

In their study of an exsolved alkali feldspar, Bollmann & Nissen (1968) suggested a parameter $P = \sum_i (b_i^2/d_i^2)$, where b_i is the magnitude of the Burgers vector of the interfacial dislocations and d_i the spacing between the dislocations constituting the ith array, as a guide to boundary energies. This parameter has been applied to phase transformations in other systems (Ecob & Ralph, 1980; Perio *et al.*, 1977; Plichta & Aaronson, 1980) including the f.c.c.–b.c.c. system. It has recently been suggested (Ecob & Ralph, 1980), by considering the homophase boundary between MoO_3 smoke crystals, treated both theoretically and experimentally by Matthews (1974, 1976), that a parameter $R = \sum_{ij} (b_i d_j/d_i d_j)^{1/2}$ is preferable to P. When the parameters P and R are applied to the f.c.c.–b.c.c. system in the N–W orientation, the parameter P predicts the most favorable interface as being approximately $(223)_F$, whereas R predicts $(0{\cdot}74, 0{\cdot}10, 0{\cdot}66)_F$ (Ecob & Ralph, 1980) for the same sets of dislocations relieving the formal interfacial Burgers-vector content. The parameter P therefore predicts the most favorable interface as being that with the minimum net Burgers-vector content for the N–W orientation, unlike the R parameter. Since experimental evidence (Hall *et al.*, 1972; Rigsbee & Aaronson, 1979*b*) tends to suggest that $(223)_F$ is a possible habit plane for the N–W orientation, it may be concluded that R is not necessarily any more useful than P, its drawback being that it will always be dominated by small d_i, *i.e.* finely spaced dislocation arrays.

Another criterion for an optimum boundary has been that $\det(\mathbf{I} - \mathbf{S}^{-1}) = 0$ (Perio *et al.*, 1977). Physically, this happens when there is perfect matching along at least one direction common to both crystals, the analogue of the invariant line in the phenomenological theory of martensitic transformations. Since, for any matrix $\mathbf{A}$, $\det \mathbf{A} = \prod_i \lambda_i$, where λ_i is the ith eigenvalue, $\mod\{\det(\mathbf{I} - \mathbf{S}^{-1})\}$ is the product of the lengths of the principal axes of the ellipsoid describing the locus of all points $\mathbf{B} = (\mathbf{I} - \mathbf{S}^{-1})\,\mathbf{p}$ for unit vectors $\mathbf{p}$. This follows from consideration of (4) and the properties of matrices. If we define $\mathbf{A} = (\mathbf{I} - \mathbf{S}^{-1})$, then the lengths of the principal axes of the $\mathbf{B}$ ellipsoid are the square roots of the moduli of the eigenvalues μ_1, μ_2 and μ_3 of the matrix $\tilde{\mathbf{A}}\mathbf{A}$. The result quoted follows, since $\det \tilde{\mathbf{A}}\mathbf{A} = (\det \tilde{\mathbf{A}})(\det \mathbf{A}) = (\prod_i \lambda_i)^2$. The optimum interface for the case when $\det(\mathbf{I} - \mathbf{S}^{-1}) = 0$ is thus the interface containing the direction of perfect matching and the direction perpendicular to it of best fit. However, this criterion and the more general one of the optimum interface being that with minimum net Burgers-vector content suggested here both necessarily fail to distinguish between the energies of the two possible dislocation descriptions of the MoO_3 interfaces and will be dominated by very coarsely spaced dislocation arrays if we consider the product $|\mu_1 \mu_2|^{1/2}$, $(\mu_1, \mu_2, < \mu_3)$ only.

We therefore conclude that none of these criteria have general applicability in indicating relative boundary energies, since the P criterion will be dominated by small d_i, whereas the $\det(\mathbf{I} - \mathbf{S}^{-1}) = 0$ criterion will be dominated by large d_i. Instead, we suggest a parameter based on the values of the principal axes of the ellipse describing the Burgers-vector content of a particular interface. Let the principal axes be $\mathbf{B}_1$ and $\mathbf{B}_2$ crossing perpendicular vectors $\mathbf{p}_1$ and $\mathbf{p}_2$ in the interface and let $\mathbf{B}_1 = \mathbf{b}_1/d_1$ and $\mathbf{B}_2 = \mathbf{b}_2/d_2$, where $\mathbf{b}_1$ and $\mathbf{b}_2$ are the individual Burgers vectors of dislocations in arrays of spacings d_1 and d_2, respectively. If we take the energy per unit length of these arrays as proportional to

$$\frac{b_i^2}{d_i}\left(1 - \ln\frac{b_i}{d_i}\right)$$

by appealing to the Volterra-type dislocation analysis of Brooks (1952), then the energy per unit area will be of the order

$$F = |\mathbf{B}_1| + |\mathbf{B}_2| - |\mathbf{B}_1| \ln|\mathbf{B}_1| - |\mathbf{B}_2| \ln|\mathbf{B}_2|, \quad (12)$$

further assuming $|\mathbf{b}_1| \sim |\mathbf{b}_2|$ and neglecting any interaction terms. The interface with minimum Burgers-vector content will therefore be also that of minimum F in this model. This equation, when used for the $(111)_F \| (110)_B$ epitaxial interfaces of Bruce & Jaeger (1978), yields the same conclusions as the criterion of Bruce & Jaeger but is influenced, rather than dominated, by the Burgers-vector content along the direction of best fit.

For the case of MoO_3 crystals, $\mathbf{B}_1$ and $\mathbf{B}_2$ have magnitudes $|f - \varphi|$ and $(f + \varphi)$ for a rotation of φ rad away from epitaxy where $f = 2(a_O - b_O)/(a_O + b_O)$ and where a_O and b_O are the lattice parameters of the a and b axes of the orthorhombic crystals (Matthews, 1974). Equation (12) then suggests that the energy per unit area of the (001) interface at φ will be of the order

$$F = (f + \varphi)\{1 - \ln(f + \varphi)\} + |f - \varphi|\{1 - \ln|f - \varphi|\}. \quad (13)$$

In particular, when $\varphi = 0$ and $\varphi = \pm f$, F has values

$$F_0 = 2f(1 - \ln f)$$

$$F_{\pm f} = 2f(1 - \ln 2f),$$

and since $f < 1$, $F_0 > F_{\pm f}$. The parameter F suggests that the orientation $\varphi = \pm f$ is energetically favorable (for $f = 0{\cdot}07$, $F_f/F_0 \sim 0{\cdot}8$), which is consistent with the experimental evidence (Matthews, 1976). However, this parameter does not differentiate between the energies of the various possible dislocation geometries for a given value of φ.

The preceding discussion has shown that the surface dislocation approach provides a quantitative measure of the misfit in an interface. In turn the lattice misorientations and interface plane orientations which correspond to minimum misfit can be calculated knowing only the appropriate lattice parameters. The misfit is expressed as a Burgers-vector density. However, nothing can be said explicitly about the structure of the interfaces concerned without knowledge in addition to that of lattice parameters and other crystallographic variables. As yet there are generally insurmountable difficulties in proceeding from a knowledge of Burgers-vector density to an absolute estimate of the elastic contribution to the interfacial energy and an explicit description of interface structure except for the case of low-angle boundaries.

It is necessary, for example, to know more about the occurrence of stable interphase boundaries analogous to special grain boundaries and allowed Burgers vectors and to take account of the difference in elastic properties of the two phases. It is expected that high-resolution transmission electron microscopy and computer modeling will be valuable in these areas. However, as a means of *comparing* the energies of interfaces which are similar with respect to elastic and chemical properties and also allowed Burgers vectors, the surface dislocation approach is very successful; this is evidenced by the breadth of experimental data which can be rationalized. No account is taken of the influence of kinetic factors which, for example in the case of epitaxial boundaries, results in the incorporation of dislocations which are not the most efficient in accommodating misfit. Similarly, modification of interfacial energy by segregation is neglected.

5. Summary

Experimental results and theoretical models of the structure and orientations of f.c.c.–b.c.c. interfaces have been analyzed with formal surface dislocation theory. The analyses suggest that the preferred interface orientations are those of minimum or close to minimum Burgers-vector contents for the Bain correspondence between the two phases. A simple semi-quantitative model has been suggested to link this concept with parameters used as guides to interfacial energies.

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